netlognews

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab NATIONAL ENERGY TECHNOLOGY LABORATORY

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netlog is a quarterly newsletter, which highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

Argonaut Jaclyn Martin helps Larry Shadle (far left) load polyethylene beads into the feed hopper of the cold flow simulator as fellow Argonauts Tim West (center left) and Hiyam Añorve Garza (center right) and teacher Melissa Hall (far right) watch. The students learned how to observe and measure the direction, velocity, and flow rate of particles in a reactor.)

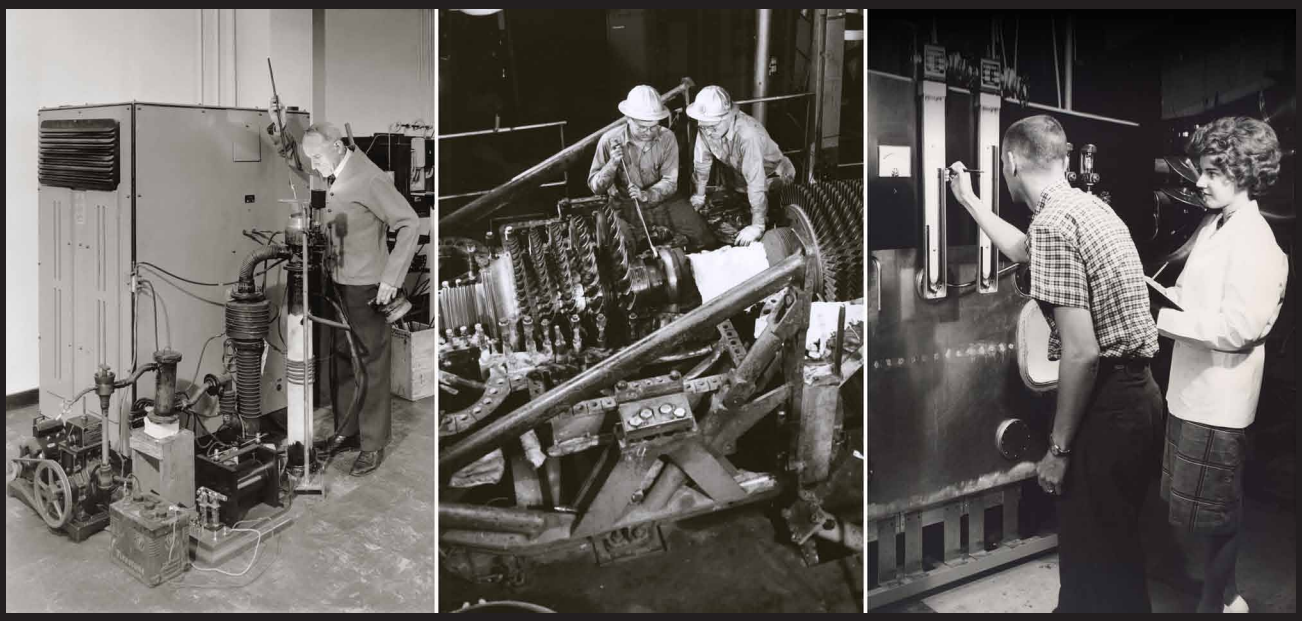
JASON Project Collaboration Yields 3 CODiE Awards

The JASON Project's multimedia energy curriculum unit developed with NETL assistance, *Operation: Infinite Potential,* has accomplished a clean sweep by winning three coveted CODiE Awards from the Software & Information Industry Association (SIIA). Representing the industry's sole peer-recognition awards program, CODiE Awards celebrate excellence and vision in educational technology, digital content, and software. The SIIA pool of educators and technology experts recognized *Operation: Infinite Potential* as the nation's Best K-12 Instructional Solution, Best Online Instructional Solution, and Best Education Game or Simulation for 2010.

Founded by the National Geographic Society, the JASON Project puts student "Argonauts" in contact with practicing explorers and researchers to excite the students about learning science. Resulting curricula become available through print, video, games, and free online resources to tens of thousands of teachers and millions of students in the United States and worldwide. *Operation: Infinite Potential* empowers students to work alongside leading scientists to explore past, current, and future challenges in energy generation, storage, and consumption. This summer, JASON released its geology unit, *Operation: Tectonic Fury,* another JASON/NETL collaboration, and is discussing a third JASON/NETL collaboration on *Forces & Motion* to be released in 2011.

Contact: Michael Nowak, 412-386-6020

100 YEARS OF INNOVATION



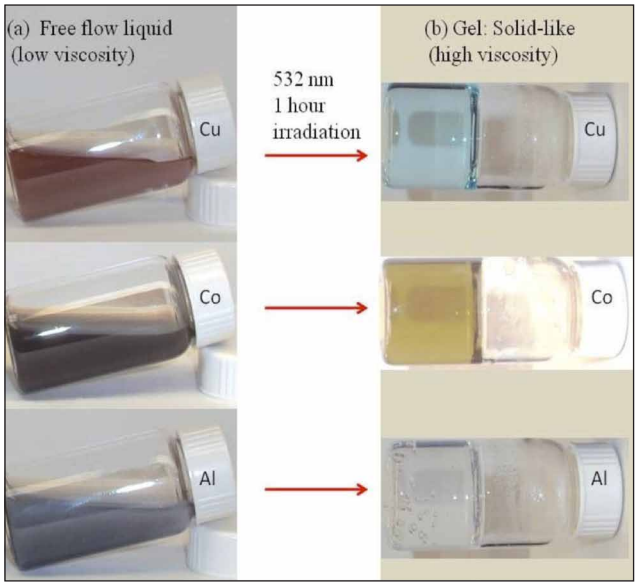
NETL Celebrates 100 Years of Research Excellence

On May 16, 1910, the newly created U.S. Bureau of Mines established the Pittsburgh Experiment Station—NETL's first predecessor organization— to improve mine safety. Since then, our laboratory has evolved from a regional organization with a single focus into a multi-faceted, multi-site national laboratory devoted to supporting the Department of Energy's mission to advance the national, economic, and energy security of the United States.

Over the last 100 years, NETL has tackled such diverse technology challenges as safe mining practices; air quality issues, including smog and acid rain; energy efficiency in our power plants, homes, and businesses; low-impact coal utilization; recovery of hard-to-reach domestic oil and natural gas supplies; and the mining and refining of rare metals for national defense and other applications.

Today, our researchers lead the fields of energy-related computational sciences, energy system dynamics research, the exploration of geologic and environmental systems, and technology development and commercialization for advanced power production.

As NETL celebrates its past 100 years, we begin pioneering research for the next 100 years. Join us in celebrating this historic achievement. Click here to see our many contributions to mine safety and energy-related science.

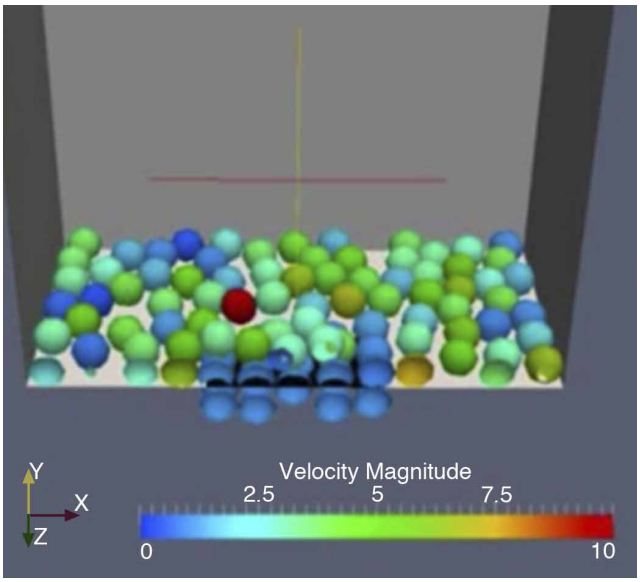


Photographs showing sol-gel transformation of aqueous solution containing 1 wt% laponite and 0.05 wt% microsized-metal powders before and after irradiation with a laser beam having fluence of 0.265 J/cm2 and wavelength of 532 nm for one hour. The solutions initially are free flow liquids with low viscosity (about 2 times higher than that of water). After one hour of irradiation the solutions became gelled when they were at rest.

NETL Develops Smart Drilling Fluids

Researchers at NETL and the University of Pittsburgh have developed hybrids of clays and iron oxide nanoparticles that can be used as rheological additives in drilling fluids. The hybrids possess unique magnetic properties unattainable in individual clay or iron oxide particles. Addition of the nanoparticles allows the rheology of water- or oil-based fluids to be finely tuned using an external magnetic field. This innovation could not only increase the efficiency of drilling operations and the longevity of drilling tools but could also find a wide range of applications in mechanical, electronic, and biomedical systems.

Contact: Phuoc Tran, 412-386-6024



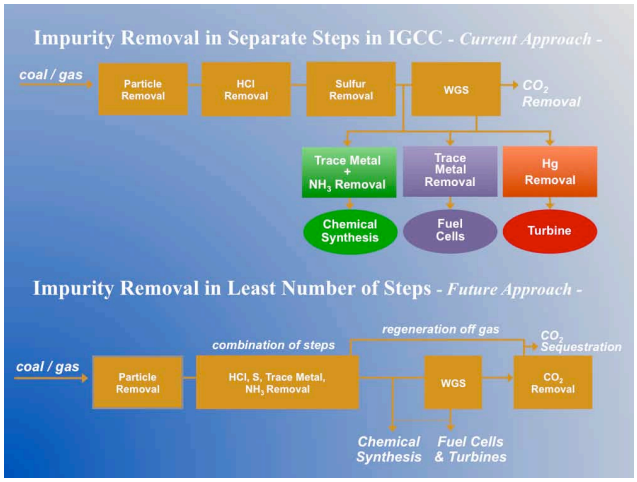
Snapshot demonstrating the new discrete mass inlet/outlet code in MFIX-DEM with a simple bottom feed case.

MFIX Code Paper Selected Best of Computing Conference Session

A paper on a Discrete Mass Inflow Boundary Condition for MFIX (Multiphase Flow with Interphase eXchanges) was selected as the best paper presented in the Computing/ Information Systems and Technology session at the SUMMER 8th International Conference on Computing, Communications, and Control Technologies (CCCT 2010).

The discrete element method (DEM) package of the NETL-developed computational fluid dynamics code MFIX was updated to handle discrete mass inlet and outlet flow boundaries. In the implementation of the discrete mass inflow boundary, any unphysical overlap between entering and existing particles is prevented, and particles entering the system will enter the computational domain regardless of opposing forces. Inflow/outflow boundary conditions are useful for simulating systems where particles are consumed through chemical reactions and an incoming feed is necessary to sustain the reaction (e.g., coal in a gasification model), or systems where particles are recycled (e.g., flow to and from a down comer in a circulating fluidized bed model). This new feature is available within the current development version of MFIX.

Contact: Janine E Carney, 541-967-5841



NETL Researchers Invent & Patent Removal Sorbent

In an effort to reduce the cost and the carbon footprint of high efficiency, coal-based power generation systems, researchers at NETL invented the first multi-functional, regenerable sorbent to simultaneously remove hydrogen chloride and hydrogen sulfide from coal gasification gas streams at warm gas temperatures of 200 to 500 °C.

Hydrogen sulfide and hydrogen chloride are major pollutants that have to be removed from the coal gasification gas streams to utilize the coal gas for various applications. After capture, the sorbent can be regenerated with oxygen. The resultant chlorine and sulfur dioxide that are formed can then be used to produce by-product liquid sulfuryl chloride, which is used in various applications including pesticide production or as a chlorine source. Multi-functional sorbents are important to minimize the cost and number of steps involved in the cleanup process.

Contact: Ranjani Siriwardane, 304-285-4513

Injection well head at a sequestration test site near Natchez Mississippi.

Storage Retention Goals for Carbon Sequestration

The effectiveness of CO_2 sequestration depends greatly on storage permanence, and consequently a key goal of NETL's carbon sequestration research program is at least 99 percent retention of CO_2 in underground reservoirs over a 100-year period. However, variability in field conditions greatly complicates quantitative leakage risk predictions.

NETL is collaborating with other U.S. Department of Energy national labs in a new effort–the National Risk Assessment Program (NRAP). The objectives of NRAP are to integrate scientific insight from across the sequestration research community and to ensure development of the science base necessary for appropriate risk assessment (including strategic monitoring) to support large-scale underground carbon storage projects. This NETL-led effort includes researchers from the Los Alamos (LANL), Lawrence Berkeley (LBNL), Lawrence Livermore (LLNL), and Pacific Northwest (PNNL) national laboratories.

After the NRAP develops its findings and recommendations, the Regional Carbon Sequestration Partnership field tests (www.fossil.energy.gov/programs/sequestration/partnerships), which are already underway, will provide ideal opportunities to apply and validate the new risk-assessment tools.

Contact: Brian Strazisar, 412-386-5988

The Multi-tube Remote Sampler shown here can sequentially expose up to 12 sampling tubes tethered to a balloon or to Unmanned Aerial Systems such as helicopters while recording exact GPS locations for each sample taken.

Novel CO_2 Monitoring Approach Field Tested

Using towers, balloons, and water wells, NETL researchers evaluated some inventive methods to detect the presence of fluorocarbon-based tracers co-injected at low levels with CO_2. These tracers can be used to fingerprint the stored CO_2, differentiating it from natural CO_2 fluxes. The use of tracers is one of the innovative methods NETL continues exploring to verify that no CO_2 leaks from carbon storage sites. A large helium-filled balloon was used to lift several carousel monitors of sealed sorbent tubes above a source of CO_2 + tracers to obtain sequential exposures of sorbent tubes at known times and known elevations to help assess boundary-layer mixing processes in the troposphere. In addition, two 8-meter towers were placed near to and 700 meters from the CO_2 release zone to sample the air at various elevations. Monitoring for atmospheric tracer plumes is expected to be a more efficient approach to leak detection than single-point subsurface measurements.

Monitoring from both the towers and balloon platform was coordinated remotely from a central control center interfaced with an on-site tower-based weather station. In a collaborative effort, NETL and USGS researchers also monitored the underground movement of CO_2 and tracers in water wells and soil-gas to exploit hydraulic gradients and changes in water chemistry as another approach to leak detection. NETL conducted the study at the Center for Zero Emissions Research and Technology experimental test facility, which is located in an agricultural field operated by Montana State University in Bozeman.

Contact: Arthur Wells, 412-386-5975

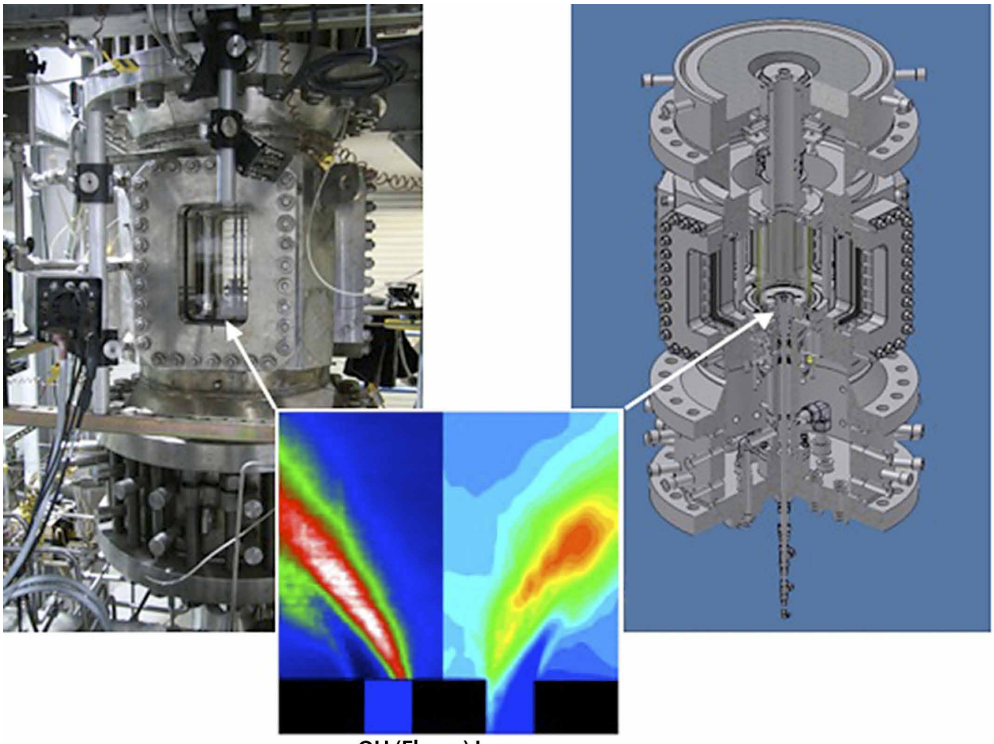
NETL Research Project Ranked 1st in an International Student Paper Competition

Doctoral student Maria Jaime, working under the guidance of NETL faculty fellow Prof. Lin at the University of Pittsburgh, has been selected as the winner in a student paper competition held at the 2010 North American Tunneling Conference, June 20-23 in Portland, Oregon. Among the papers submitted by students from Canada, Mexico, and the United States, three finalists were selected to receive a travel award to present their research at the conference. After the presentations, the committee selected Jaime as the winner and presented a prize of $1,500 to her.

Jaime's doctoral research on "Numerical modeling of the rock fragmentation process when drilling into high pressure environments using the explicit finite element method" is part of NETL's Extreme Drilling research portfolio. The project focuses on understanding and predicting the forces developed at the cutter-to-rock interface in the bottom of a well three to four miles beneath the earth. This is an integral part of NETL's research to enhance the fundamental understanding of deep drilling phenomena where temperatures and pressure exceed 200 °C and 20 kpsi.

Another doctoral student, Jorge A. Mendoza, working on the same project, received the 2010 outstanding student research paper at the American Society of Civil Engineers Pittsburgh chapter oral presentation award. The title of his presentation was "Simulation of rock cutting using distinct and crushable elements."

Contact: Isaac K. Gamwo, 412-386-6537



OH (Flame) Image
SimVal Experiment CFD Simulation

Shakedown Testing of High-Pressure Combustion Facility Completed

The NETL High-Pressure Combustion Facility houses two separate combustion test facilities:

- the Low Emission Combustor Test and Research/Simulation Validation Studies (LECTR/SimVal) facility, and the
- Dynamic Gas Turbine/Aerothermal Studies (DGT/Aerothermal) facility.

The LECTR/SimVal facility is an optically-accessible, pressurized combustion research unit which allows direct observation of combustion processes during operation at pressures to 20 atm in a controlled environment representative of commercial gas turbine combustors. This capability is used to: (1) develop and evaluate novel combustion concepts and hardware needed to increase the cycle efficiencies of and decrease the emissions from future power systems; and (2) provide high-quality validation data sets to promote the advanced Computational Fluid Dynamics (CFD) needed to develop these future power systems.

The DGT/Aerothermal facility consists of an optically-accessible combustion test section and an additional optically-accessible test section for conducting turbine aerothermal, materials and sensors research in an environment representative of gas turbine combustors at pressures to 10 atm. These capabilities can: (1) explore aerothermal protection and material issues related to future hydrogen and oxyfuel turbines; (2) enable the detailed study of heat transfer and cooling mechanisms, turbine blade materials, and thermal barrier coatings; and (3) enable the development and testing of advanced turbine sensors and instrumentation.

The data produced are expected to help develop robust turbine hardware and sensors capable of operating at temperatures higher than is currently possible, thus enabling the development of advanced power systems that would operate at higher turbine inlet temperatures and higher cycle efficiencies.

Contact: Todd Sidwell, 304-285-5452

New Research Micro-CT Scanner Outperforms Medical CT

A new laboratory micro-CT scanner, an Xradia MicroXCT-400, has the ability to reveal features down to 1 µm, in contrast to the medical CT used for many years, which has a resolution of 250 µm. Core-scale gas injection tests artificially generated fine fractures in a silt core and it was predicted that gas hydrate would form within the fractures. Fractures in the core were observed first with the medical CT scanner during the experiment simulating natural conditions and then were examined using the micro-CT scanner at ambient condition after dissociating any hydrate. The micro-CT confirmed the presence of fine cracks and cavities in fine sediments.

The new, higher resolution micro-CT scanner enabled researchers to confirm micro-fracture generation and non-linear irregular patterns of the fractures at a pixel resolution of 40 µm, which previously could have been misinterpreted as density changes based on images from the medical CT. Observing fine fractures and hydrate crystal growth within them will help to understand mechanisms by which hydrate-filled fractures form, how gas migrates through low-permeability sediments, and how large hydrate lenses form., This new tool will greatly enhance NETL's capability in other research ventures as well.

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Yongkoo Seol, 304-285-2029

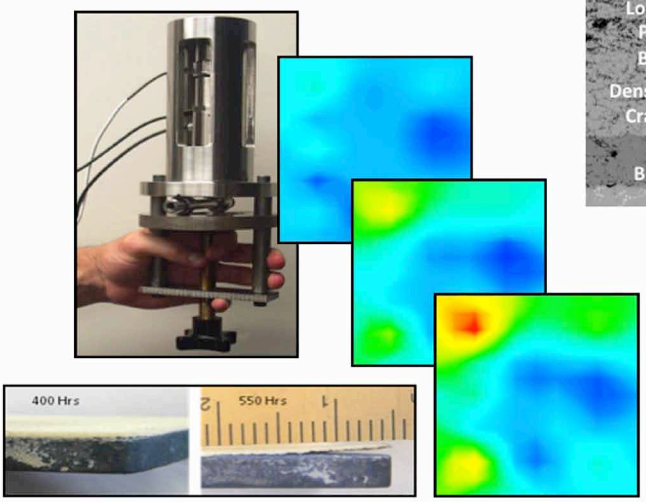
Radio-Frequency Electromagnetic Fields Enhance Catalytic Activity

For several years, NETL has been conducting research in assessing and providing fundamental information on reforming of hydrocarbon feed stocks/fuel into a hydrogen-rich synthesis gas, a necessary enabling technology for fuel cells and other applications. The potential use of radio-frequency (RF) electromagnetic fields to enhance catalytic hydrocarbon reforming was recently evaluated. Preliminary studies showed up to a 20% increase in syngas yields when RF fields were applied to a relatively non-performing reforming catalyst. Some evidence of a reduction in coke/carbon was also observed, but further testing is underway to repeat and quantify these results.

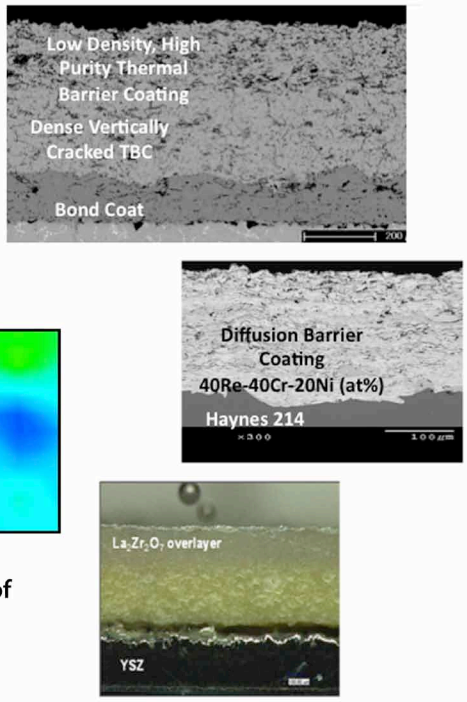
One of the major problems when reforming heavy hydrocarbons into syngas using traditional metal-based catalysts is the formation of unwanted by-products such as solid coke/carbon that can degrade the lifetime and performance of solid oxide fuel cells. The RF field appears to potentially provide a means to control how energy is dispersed into the reformer (not just through bulk heating of reactants), which can have a direct impact on energy consumption and ultimate system performance and syngas quality.

NETL will continue exploration of this effect to quantify potential and fundamental properties through precise control of RF frequency, power, catalytic properties, and process operating conditions.

Contact: Dushyant Shekhawat, 412-304-285-4634



Non-Destructive Evaluation and Life Prediction of Thermal Barrier Coatings



Advanced Coatings Development

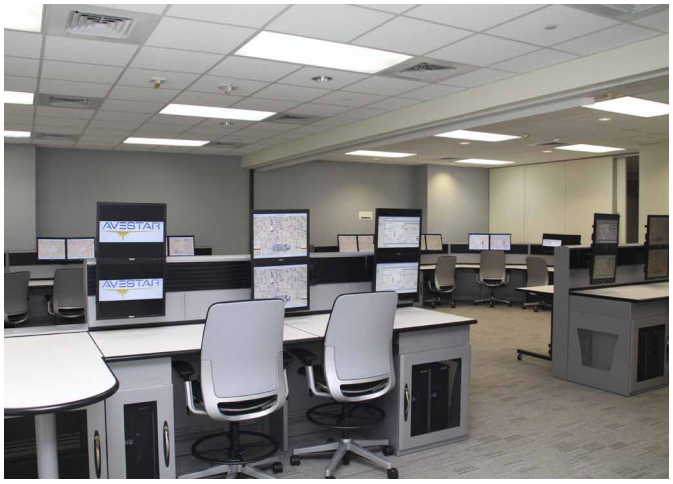
NETL and Regional University Alliance Team Develop New Materials and Non-Destructive Evaluation Techniques

NETL, the University of Pittsburgh, and West Virginia University, under the NETL-Regional University Alliance (RUA) consortium, collaboratively developed advanced turbine material systems and early failure non-destructive evaluation (NDE) prediction techniques for application to future gas turbine engines. The team demonstrated that variation in average surface stiffness measured by micro-indentation, as well as wave reflection amplitude and travel time observed by pulse-echo NDE techniques, could be used to identify the early onset of internal thermal barrier coating (TBC) debonding in bench-scale laboratory testing. And, importantly, micro-identification could be used prior to visually observing external crack formation, spallation, and loss of the TBC coating.

The success of the team's acousto-ultrasonic NDE efforts attracted a field-service supplier to provide an in-service full combustor liner to identify potential subsurface TBC debonding areas where refurbishment would be needed. Also, working in conjunction with commercial metal and coating suppliers, the team demonstrated the stability, insulating capability, and cyclic operating life of a high-purity, low-density thermal barrier coating that exceeded bench-scale performance of conventional state-of-the-art TBC coatings.

The feasibility of diffusion barrier coatings to reduce elemental interdiffusion, while retaining high-temperature oxida¬tion resistance of nickel-based super alloys, was shown. Excellent high- temperature life as compared with commercial state-of-the-art bond coat systems was demonstrated for NETL's modified, reduced-cost, diffusion bond coat system. Also, thicknesses and compositions of extreme temperature over layer coatings were projected for use in advanced land-based engines. Details of these efforts are provided in NETL's Office of Fossil Energy, Advanced Turbine Program, and Fiscal Year 2010 Turbine Annual Report.

Contact: Mary Anne Alvin, 412-386-5498



NETL's AVESTAR (Advanced Virtual Energy Simulation Training and Research) Center to be deployed in November.

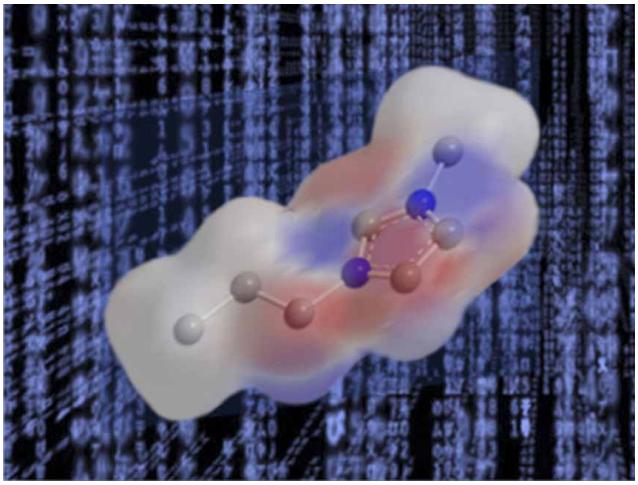
IGCC Dynamic Training Simulator Model Validated

NETL and its project partners, West Virginia University, Fossil Consulting Services, EPRI, and Invensys Operations Management, have completed two weeks of dynamic model validation for NETL's IGCC dynamic simulator and operator training system.

To validate the gasification side of the IGCC plant, the coal feed rate to the gasifier trains was slowly ramped down until emergency shutdown conditions were triggered. At that time, all equipment was isolated and shut down. From these warm shutdown conditions, the gasification trains were restarted, followed by startup of the syngas scrubbers, shift reactors, gas cooling system, sour water stripper, dual-stage Selexol process for capture of hydrogen sulfide and CO_2, Claus plant, and CO_2 compression. As an additional dynamic test, the coal feed to the IGCC plant was transitioned from Illinois #6 coal to a mixture of Illinois #6 subbituminous and West Virginia bituminous coal.

The combined cycle side of the IGCC plant was validated with a startup from cold conditions, followed by a transition to syngas and full load. Both gas turbines were then ramped down, transitioned back to natural gas, and put through a controlled shutdown. The system will be deployed in November 2010 at NETL's AVESTAR (Advanced Virtual Energy Simulation Training and Research) Center.

Contact: Stephen E. Zitney, 304-285-1379



NETL Sensor Research Featured in a New Book

A recently published book, Trends in Photonics, includes a chapter "Photonic-Bandgap-Fiber Sensors for Gas Detection," that was written by Michael Buric, Kevin Chen, Joel Falk, and Steven Woodruff of NETL. This chapter focuses on their early work studying the use of photonic bandgap optical fibers as gas sensors utilizing Raman spectroscopy. The chapter was written at the invitation of the editor, Prof. John Canning of the Interdisciplinary Photonics Laboratories, University of Sydney, who produced the book for Research Signpost, Kerala, India. The authors are research colleagues in a Regional University Alliance project that is developing a gas sensor for natural gas, syngas from coal gasification, and biogas from landfills and biodigestion. The sensor can monitor all species in these gases with a onesecond time response.

Contact: Steven Woodruff, 304-285-4175

NETL Licenses Patented Technology to International Instrument Manufacturer

Officials at NETL and Zolo Technologies, Inc., have signed a Memorandum of Understanding to license and use NETL-patented transpiration probe. The probe can stay cool and maintain clean optical surfaces while allowing optical access to high-temperature,

hazardous, and dirty environments for extended periods. Zolo Technologies plans to incorporate the technology into laser-based ZoloBOSS sensors, which can see through flame, dust, and ash to measure multiple constituents in the harshest environments, including coal-fired combustion processes.

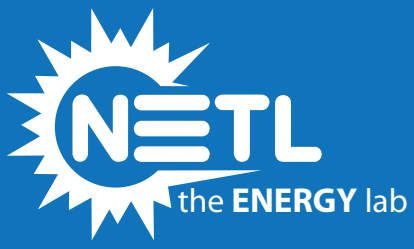
Contact: John VanOsdol, 304-285-5446

Patents Issued

1.	Alvin, Mary Anne, "Thermal Barrier Coatings," US Patent 7,740,948, issued June 22, 2010.
2.	Siriwardane, R., "Regenerable Hydrogen Chloride Removal Sorbent and Regenerable Multi-Functional Hydrogen Sulfide and Hydrogen Chloride Removal Sorbent for High Temperature Gas Streams," US Patent 7,767,000, issued August 3, 2010.
3.	Granite, Evan J., and Henry W. Pennline, "Catalysts for Oxidation of Mercury in Flue Gas," US Patent 7,776,780, issued August 17, 2010.

Recent NETL Publications

1.	Baltrus, John P. and Evan J. Granite, Henry W. Pennline, Dennis Stanko, Hugh Hamilton, Liz Rowsell, Stephen Poulston, Andrew Smith, Wilson Chu, "Surface characterization of palladium–alumina sorbents for high-temperature capture of mercury and arsenic from fuel gas," *Fuel*, 2010, (89), pp1323-1325.
2.	Shi, Wei and Dan C. Sorescu, David R. Luebke, Murphy J. Keller, Shan Wickramanayake, "Molecular Simulations and Experimental Studies of Solubility and Diffusivity for Pure and Mixed Gases of H_2, CO_2, and Ar Absorbed in the Ionic Liquid 1-n-Hexyl-3-methylimidazolium Bis (Trifluoromethylsulfonyl)amide ([hmim][Tf_2N])," *The Journal of Physical Chemistry B*, 2010, 114 (19), pp 6531-6541.
3.	Rupp, Erik C., Evan J. Granite, and Dennis C. Stanko, "Method for Detection of Trace Metal and Metalloid Contaminants in Coal-Generated Fuel Gas Using Gas Chromatography/Ion Trap Mass Spectrometry," *Analytical Chemistry*, Vol. 82, No. 14, July 15, 2010.
4.	Pennline, Henry W. and Evan J. Granite, David R. Luebke, John R. Kitchin, James Landon, Lisa M. Weil, "Separation of CO_2 from flue gas using electrochemical cells," *Fuel* (2010) 891307-1314.
5.	Uguz, A. Karem and Mehrdad Massoudi, "Heat Transfer and Couette Flow of a Chemically Reacting Non-linear Fluid," *Mathematical Methods in the Applied Sciences*, 2010, 33 (11), pp 1331-1341.
6.	Brown, Thomas D. and Charles E. Taylor, Mark P. Bernardo, "Rapid Gas Hydrate Formation Processes: Will They Work?." Energies 3, 2010, no. 6: pp. 1154-1175.
7.	Shekhawat, D. and D. Berry, H. Pennline, E. Granite, J. Spivey, (Guest Editors), Preface - Advanced Fossil Energy Utilization, Fuel, 89, June 2010, pp. 1185-1186.



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